Supporting information

Block copolymer-coated ATR-FTIR spectroscopic sensors for monitoring hydrocarbons in aquatic environments at high temperature and pressure

Charles Heath*, Bobby Pejcic and Matt B Myers

CSIRO, Energy, 26 Dick Perry ave, Kensington, WA, 6151, Australia

*Corresponding author Tel: +61 8 6436 8922, Fax: +61 8 6436 8555, E-mail address: Charles.Heath@csiro.au.

Polymer film surface characterization

To investigate the thermal stability of Kraton G-1650, a film was made on a glass slide was subjected to different temperatures and images collected using an optical microscope (Figure S1). 10µl of a solution of Kraton G-1650 in $CHCl_3$ (10mg/mL) was dropped onto a glass slide and allowed to dry for 2 hours. This polymer film was then photographed using a Nikon eclipse LV100N POL optical microscope at 25x magnification. The same glass slide was then placed into pure water for 24 hours at 22°C, removed and allowed to dry and photographed again in the same area. This was repeated at different temperatures.

FTIR of polymer films at different temperatures

FTIR spectra of polymer films in the absence of aqueous solutions between 22-80°C and ambient pressure were recorded using the Bruker Alpha with diamond ATR (Figures S2 and S3). The diamond ATR is equipped with a heater and thermocouple controller that may be adjusted using the software OPUS. A new background was acquired at each temperature and a polymer film was then drop cast onto the diamond (10µl of a 50mg polymer in 5ml $CHCl_3$ solution). The film was allowed half an hour to stabilize at the required temperature and the spectrum then recorded.

Table S1 Parameters of linear regression for the toluene calibrations of the various polymer flims studied.

Toluene	Styrene/Isoprene	Styrene/butadiene	Kraton G-1650	PIB
Intercept	-0.0043 ± 0.004	-0.0007 ± 0.003	-0.00012 ± 0.007	-0.0016 ± 0.006
Slope	0.0039 ± 0.0002	0.0027 ± 0.0002	0.0069 ± 0.0004	0.0039 ± 0.0003
R^2	0.99	0.99	0.99	0.99

Table S2 Parameters of linear regression for the toluene and napthalene calibrations of Kraton G-1650 at 137 bar, 22-80°C.

Toluene	22°C	40°C	60°C	80°C	22°C repeat
Intercept	0.0077 ± 0.016	0.0068 ± 0.013	0.0031 ± 0.010	0.0127 ± 0.004	0.0046 ± 0.007
Slope	0.0148 ± 0.0006	0.0122 ± 0.0005	0.009 ± 0.0004	0.0016 ± 0.0001	0.0047 ± 0.0002
R^2	0.99	0.99	0.99	0.99	0.99
Naphthalene					
Intercept	-	0.0146 ± 0.025	0.0063 ± 0.014	0.0153 ± 0.005	-
Slope	-	0.0749 ± 0.0054	0.0411 ± 0.0029	0.0096 ± 0.0008	-
R^2	-	0.99	0.99	0.99	-

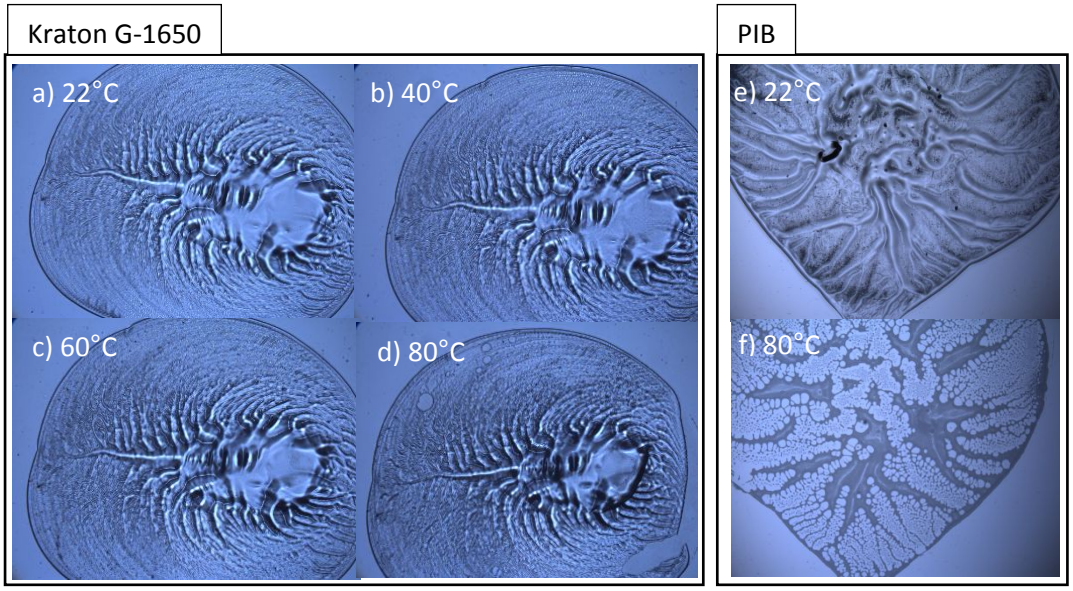

Figure S1 Optical images of a Kraton G-1650 drop cast film after exposing it to water for 24 hours at: a) 22°C b) 40°C c) 60°C d) 80°C at 1 bar (left) and optical images of a PIB drop cast film after exposing it to water for 24 hours at: e) 22°C f) 80°C at 1 bar (Anal. Chem. 2017, 89, 13391−13397).

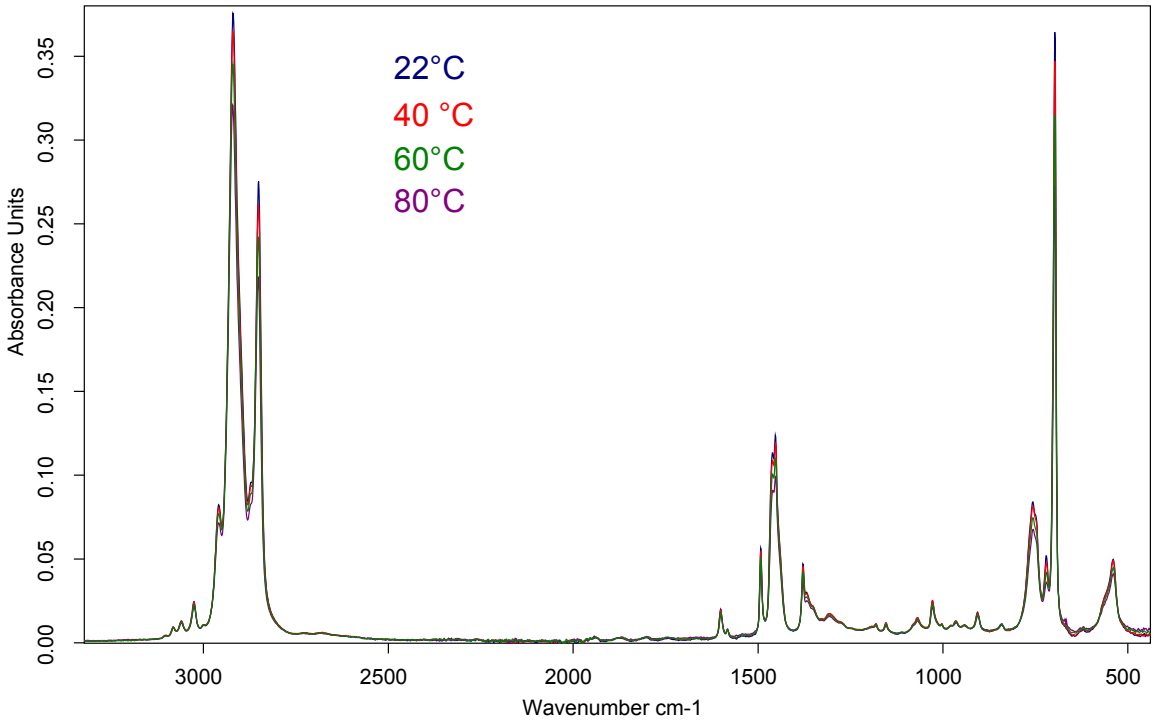

Figure S2 FTIR spectra of Kraton G-1650 recorded at 22, 40, 60 and 80°C at ambient pressure in the absence of aqueous solutions.

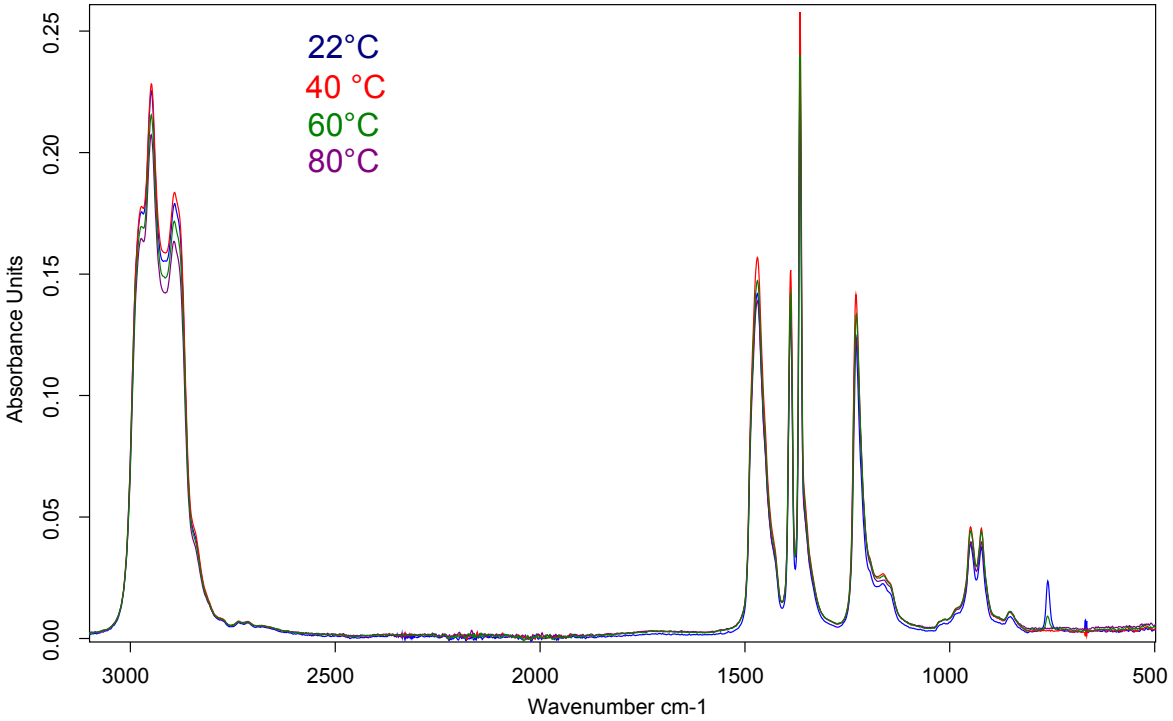

Figure S3 FTIR spectra of pure polyisobutylene recorded at 22, 40, 60 and 80°C at ambient pressure in the absence of aqueous solutions. Peak at 761cm^{-1} is due to residual $CHCl_3$.